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New User Orientation

Introduction

The NAS New User Orientation guide gives first-time users a brief overview of the high-performance computing (HPC) environment operated by staff in the NASA Advanced Supercomputing (NAS) facility at Ames Research Center, Moffett Field, California. It contains all the basic information you must know to get started with using the supercomputing resources and services provided at the facility. Returning users may find the guide useful as a quick refresher.

Throughout this guide you will find links to other NAS Knowledge Base articles to help you become familiar with some of the details needed to navigate the complex NAS environment. You can also use the Knowledge Base to browse FAQs and search for other topics of interest. The resources within the NAS environment are funded through NASA's High-End Computing Capability Project, and the terms "NAS" and "HECC" are used interchangeably throughout the Knowledge Base.

The guide includes the following basic topics:

- **Introduction**: Covers what you need to know before you begin, some reminders about your responsibilities as a NAS user, and typographic conventions used
- **Environment Overview**: Describes the general setup of the NAS/HECC secure environment, the computer, network, and data storage components, and the user environment
- Basic Tasks: Provides a general description of the tasks that comprise a typical user workflow
- **Understanding and Managing Your Allocations**: Summarizes how computing time is calculated, tracked, and charged
- **Helpful Resources**: Provides links to help you find more information, and summarizes additional services that are provided by NAS experts

If you still can't find the information you're looking for, the NAS Control Room staff are available 24x7 to provide additional help.

Toll-free Telephone: 800-331-8737 Local Telephone: 650-604-4444 E-mail: support@nas.nasa.gov

Before You Begin

To make the best use of this guide and to perform basic tasks, you must already have done the following:

- Received approval for your request for allocation
- Completed the two-phase user accounts process for NAS systems
- Received your <u>RSA SecurID fob</u> for two-factor authentication
- Obtained your password and enabled your RSA SecurID fob

If you need assistance with any of these items, call the NAS Control Room at the telephone number shown above.

User Responsibilities

New User Orientation 1

When you completed your Account Request Form, you agreed to abide by a set of rules by signing NAS's <u>Acceptable Use Statement</u>. Below are a few basic reminders.

- The computing systems are unclassified systems; classified information may not be entered, processed, or stored
- Users cannot divulge access information (for example, lists of user accounts)
- Users cannot share their account(s) with anyone, including sharing account passwords, providing access via a .rhost entry, or any other means of sharing--if you are found sharing accounts, your accounts will be disabled
- It is your responsibility to become familiar with various NASA security-related policies

Conventions Used in This Guide

The following table shows the typographical conventions used in this guide.

Convention	Description	Examples
Percent sign (%)	Indicates the system prompt; your system prompt may be different	pfe <i>20</i> % Local%
Monotype	Indicates commands	Run the command mylou
Italicized words or phrases	Indicate command variables; variable number ranges; substitute your own phrase; rarely, indicates emphasis or introduces a new term	tbd pfe[20-27] your_username Never share your password. The hotspots analysis
Bold	Indicates man pages to reference	Read the ifort man page for more information

Introduction 2

Helpful Resources

You can find additional information such as important user announcements and training sessions from the following links:

- NASA High-End Computing Capability (HECC) News
- HECC Frequently Asked Questions
- System Status
- HECC User Training
- Past Webinars Archive
- NASA Advanced Supercomputing (NAS) Division

Remember that NAS Control Room staff are available 24 hours a day, seven days a week:

Toll-free Telephone: 800-331-8737 Local Telephone: 650-604-4444 E-mail: support@nas.nasa.gov

The following support services are also offered free of charge to all users:

- Application performance optimization and code porting
- End-to-end network services for troubleshooting and performance
- Customized training and support to help users efficiently manage large amounts of data
- Advanced scientific visualization and analysis capabilities

For more information about our service offerings, see <u>HECC Services Overview</u>.

Helpful Resources 3

Basic Tasks

Once you have completed preliminary tasks and read the <u>Environment Overview</u>, you can get started with using the supercomputers. The basic tasks below cover a typical user workflow cycle.

Even these basic tasks require numerous setup steps before you can perform specific tasks on the supercomputers. For each task, follow the links provided below to other Knowledge Base articles to get step-by-step instructions and more details on our HPC environment.

Logging in for the First Time

Once you have obtained your default NAS password and enabled your RSA SecurID fob, you must complete a series of steps to be able to log into the supercomputers. If you have not yet obtained your default password and enabled your RSA SecurID fob, please see <u>Before You Begin</u>.

After you log in for the first time, subsequent logins will be more straightforward. The first time you access a system in the secure enclave, you will log into one of the secure front-end (SFE) systems, designated sfe[1-4], as shown in the <u>environment overview diagram</u>. You will complete two-factor authentication using the your fob and your NAS password. For step-by-step instructions and examples, see <u>Enabling Your SecurID Fob and First-Time Login</u>.

Note: The secure front-end systems are used only as gateways to the enclave resources and are not to be used for storing data. You can store data in your Pleiades home directory, your /nobackup directory, or on your Lou directory.

Subsequent Logins

Once you successfully log in for the first time, your subsequent logins can be done using either a two-step connection method or a one-step method, both of which require the use of your fob and connection through the SFEs.

TIP: Use the one-step connection method described below. This method takes more time to set up, but saves time in the long run.

Two-step Connection

Initially, you may want to use the two-step connection method, which involves connecting from your desktop to the SFEs and then to resources within the secure enclave, without setting up the SSH passthrough feature. However, this method can be cumbersome and time-consuming if you use several logins. You can choose two options for this approach: one uses your NAS password and RSA SecurID passcode; the other requires that you first set up public key authentication. For instructions and examples, see the following articles:

- Two-Step Connection Using SecurID Passcode and NAS Password
- Two-Step Connection Using Public Key and SecurID Passcode

One-step Connection

With this method, you can bypass logging into an SFE each time by using SSH-tunneling to transparently "pass through" the SFEs. The SSH passthrough feature allows you to log into any system in the enclave by typing just one SSH command. To set up one-step connection, you will first set up public key authentication and SSH passthrough. Once these steps are completed, you can access any of the systems in what appears to be a single step. For step-by-step instructions and examples, see the following articles:

- 1. Setting Up Public Key Authentication
- 2. Setting Up SSH Passthrough
- 3. One-Step Connection Using Publickey and Passthrough

Transferring Files From Your Local System to NAS Systems

You can choose from several different methods to transfer files from your local system to your directories within the secure enclave. Remote file transfer methods and commands such as sup/shiftc, scp, bbftp, and bbscp are supported on most NAS systems. You may need to install the client and/or server software for the SUP/Shift client, SCP, bbFTP, or the bbSCP script on your local host in order to use these methods.

TIP: Use the **shiftc** command to transfer files from your local system to NAS systems. This command dynamically selects the highest performing transfer method available, and is normally the optimal tool for transferring files of any size.

When you initiate file transfers from your local system to the NAS systems, you will be prompted for your SecurID passcode. (You may then be prompted for further authentication, depending on whether you have set up SSH passthrough.) File transfers that are initiated from the NAS systems to your local system might be a simpler way to transfer files, if your local system does not require two-factor authentication. For more information, see the following articles:

- Remote File Transfer Commands
- Shift File Transfer Overview

Below are examples of initiating **shiftc**, **scp**, and **bbftp** from your local system. The examples assume that you have downloaded the SUP client and bbFTP script, and that your username for your local system is different than your username for the NAS systems.

Note: If your local host username and your NAS username are the same, you can omit *nas_username@* from the command line.

shiftc example

```
your_local_system% sup -u nas_username shiftc lou.nas.nasa.qov:filename ./filename
```

scp example

```
your_local_system% scp nas_username@lou.nas.nasa.gov:filename ./filename
```

bbftp example

```
your_local_system% bbftp -u nas_username -e 'setnbstream 2;
get filename' -E 'bbftpd -s -m 2' lou.nas.nasa.gov
```

Compiling Your Code

Several compilers and tools for major programming languages are available on the NAS systems. Because there is no default compiler, you must load a compiler module. Use the module avail command to view all available modules.

Note: NAS recommends using Intel compilers for building your applications on Pleiades, Electra, Endeavour, or Merope. Available modules include Intel compilers for both Fortran and C++.

You can use the following commands to invoke the various versions of Intel compilers:

```
ifort
Intel Fortran
icc
Intel C
icpc
Intel C++
```

For example, to compile the application *filename.f* with ifort, type:

```
% ifort filename.f
```

Read the **ifort**, **icc**, and **icpc** man pages for options to use. Type **man** *topic* to access the man page for any particular topic. See <u>Intel Compiler</u> for more information.

Note: Because Pleiades and Merope are running different operating systems, an executable file built on Pleiades may need to be recompiled on Merope.

Porting and Running MPI Codes with SGI's MPT Library

SGI's Message Passing Interface (MPI) is a component of the Message Passing Toolkit (MPT), which supports parallel programming across a network of computer systems. To use MPI, you must first load an Intel compiler module and an SGI MPT module on Pleiades, Electra, Endeavour, or Merope. The example below shows how to compile and link your code with MPT:

```
% ifort -o filename filename.f -lmpi
```

To run your MPI codes with MPT in a PBS job, insert the following in your PBS script, where *xx* represents the number of MPI processes:

```
mpiexec -np xx filename
```

For more information about using MPI and MPT, see <u>SGI MPT</u>. For a comprehensive overview of compiling and porting code, see the articles listed in <u>Porting and Developing Overview</u>.

Submitting and Running Jobs

Once you have completed the basic setup, transferred your files to the NAS systems, and compiled your code, you're ready to run jobs on the compute nodes.

NAS facility supercomputers use the Portable Batch System (PBS) from Altair Engineering, Inc., for job submission, monitoring, and management. You can run a job through an interactive session using PBS, or you can submit batch jobs by using a PBS job script. In either case, all jobs are submitted to PBS by issuing the gsub command from the PFEs or from the Merope front-end system.

For more information about PBS, see <u>Portable Batch System (PBS) Overview</u>. For more information about all of the PBS commands described in the following sections, see <u>Commonly Used PBS Commands</u>.

Submitting Interactive (Single) Jobs

To run a job interactively, use the PBS command **qsub** -I (interactive). On the command line, you can request specific resources by using the -1 (liquid) option. For example:

```
pfe20% qsub -I -lselect=1:ncpus=8,walltime=1:00:00
```

In the above example, the user submits a job to Pleiades from pfe20, requesting 1 node with 8 cores and 1-hour maximum wall-clock time. To submit the same job and resource request to Endeavour, specify the Endeavour PBS queue, pbspl3, on the command line:

```
pfe20% qsub -I -lncpus=8 -q @pbsp13
```

To submit the same job and resource request to the Merope compute nodes, submit the job from the Merope front end:

```
mfe1% qsub -I -lselect=1:ncpus=8, walltime=1:00:00
```

Submitting Batch Jobs

Before submitting a batch job, you must first create a PBS job script. The following sample script uses the select option to request 4 nodes with 8 cores per node and 1 hour of maximum wall-clock time.

```
#PBS -1 select=4:ncpus=8
#PBS -1 walltime=1:00:00
cd $PBS_O_WORKDIR
mpiexec -np 32 ./a.out
#end of script
```

Now, you can submit the batch job to run on the Pleiades, Electra, Endeavour, or Merope compute nodes. For example, to submit this job from pfe 20 to Pleiades, issue the following command:

```
pfe20% qsub job_script
```

To submit this job from pfe20 to Endeavour, specify the Endeavour PBS queue, pbspl3, in the command line:

```
pfe20% qsub -q @pbspl3 job_script
```

To submit this job to the Merope compute nodes, submit the job from the Merope front end:

```
mfel% qsub job_script
```

Monitoring Jobs

When you submit a job to PBS, it is assigned a job identification number (JOBID). PBS jobs are usually in either the Running (R) state or the Queued (Q) state. Use the following commands to find the status of your jobs, using JOBID 12345 as an example:

```
show the status of your jobs

qstat -nu nas_username
list all jobs that belong to you

qstat 12345
check the status of a job

qstat -f 12345
check the status of a job (with full details)

qstat -s 12345
show why a job is not yet running
```

You can also monitor your jobs using the myNAS mobile app, which enables you to view job status, receive

notifications when jobs change state or produce output, and view output files on your iOS or Android device. For more information, see the following articles:

- Installing the myNAS Mobile App
- Using the myNAS Mobile App

Managing Jobs

If you need to delete a job or place it on hold, use the following PBS commands, which use JOBID 12345 as an example:

```
qdel 12345
delete a job
qhold 12345
place a job on hold
qrls 12345
release a job from hold
```

For troubleshooting information, see the following articles:

- Common Reasons for Being Unable to Submit Jobs
- Common Reasons Why Jobs Won't Start

Managing Your Data

Managing the data that your jobs use and create is an integral part of computing at NAS. At different times you may need to transfer data to/from NAS to your remote site, check your disk use and quotas, copy files from the Lou tape drives, or share files with other NAS users. For more information, see the following articles:

- Remote File Transfer Commands
- Pleiades Home Filesystem
- Pleiades Lustre Filesystems
- The dmget Command
- Using 'Giveto' to Copy Files and/or Directories to Another User

Checkpointing Jobs

A checkpoint is a snapshot of your job taken periodically while it is running. If the job runs out of wall-clock time or fails for any reason, it can be restarted from the checkpoint. Be aware that none of the HPC operating systems have an automatic checkpoint capability. Therefore, for jobs that need a lot of resources and/or long wall-clock time, we recommend implementing a checkpoint/restart capability in your source codes or job scripts.

In the event that an HPC system crashes or experiences certain system issues, PBS automatically reruns jobs when the system is back up and issues are resolved. If you do not want PBS to rerun your job, add the following line to the top of your PBS script:

#PBS -r n

Storing Your Files

To ensure your data is stored securely, and to maintain directory space and avoid quota limits, you will periodically transfer your files from the scratch/nobackup directory and the compute nodes to the Lou mass storage systems.

The scratch /nobackup filesystems are mounted on Lou, enabling disk-to-disk copying, which provides the highest transfer rates. You can use the commands shifte, cp, or mcp to copy files or make tar files directly from your scratch/nobackup directory to your Lou home directory. Note that Pleiades, Electra, Endeavour, and Merope share the same home and /nobackup filesystems.

Network file transfers to the Lou systems are sent through the 10 GigE interface by default. You can use the commands **shiftc**, **scp**, **bbftp**, and **bbscp** to transfer your files. NAS recommends using **shiftc**, as it dynamically selects the highest performing transfer method available.

File transfers from the compute nodes to Lou must first go through the front-end nodes (PFEs for Pleiades, Electra, and Endeavour; mfe1 for Merope) or through the /nobackup filesystems. For more information, see the following articles:

- Local File Transfer Commands
- The Lou Mass Storage System

TIP: When sending data to Lou systems, keep your largest individual file size under 1 TB, as large files will keep all of the tape drives busy, preventing other file restores and backups.

Post-Processing Your Data

After your work has completed running on the compute nodes, you can perform post-processing tasks on the <u>Lou data analysis nodes</u>.

The NAS hyperwall visualization system provides a supercomputing-scale resource to process very large datasets produced by the HPCs, and NASA scientific instruments. Although general users cannot access the system, our visualization experts provide post-processing services. For an overview of the system, see <u>Visualization System: hyperwall</u>.

Understanding and Managing Your Allocations

As part of applying for a NAS account, you (or your principal investigator) requested an allocation for computing time on Pleiades, Endeavour, or both. Allocations for NAS supercomputing resources are granted per project ID number (GID), and are specified in standard billing units (SBUs). If you have a Pleiades allocation, you can run jobs on both Pleiades and Merope.

Usage Charge Methods

System usage is charged as follows:

- Front-End Systems: Usage is *not* charged on the Pleiades front-end systems (PFEs) or the Merope front-end system (mfe1). However, remember that these front-end nodes are intended for editing and/or compiling and running short testing jobsâ not for running production jobs. If you misuse these systems, your jobs will be terminated.
- Lou Data Analysis Nodes: Usage is *not* charged on the Lou data analysis nodes (LDANs), which provide dedicated PBS resources for pre- and post-processing tasks.
- Compute Nodes: Usage on the Pleiades, Merope, and Endeavour compute nodes is charged. The number of SBUs charged to a job is calculated by multiplying the number of total wall-clock hours used by the minimum allocation units (MAUs)â the smallest unit of hardware resource that the Portable Batch System (PBS) will allocate to a job.

SBU rates vary by processor type, as follows:

	Host	SBU Rate
	Broadwell	4.04
Pleiades	Haswell	3.34
	Ivy Bridge	2.52
	Sandy Bridge	1.82
Merope	-	1.00
Endeavoi	ur	0.74

Note: When your allocation has been expended, you will no longer be able to run jobs, and you will need to request more hours. You can check your remaining SBU balance by running the command acct_ytd on the system(s) where you have accounts.

For more information, see the following articles:

- Standard Billing Units (SBUs)
- Job Accounting
- Job Accounting Utilities

Charging to a Non-Default GID

If you have access to more than one GID, only one of those GIDs is set as your default. The default GID is listed in the /etc/passwd file of each system you have access to. Your jobs will be charged to the default GID unless you specify a different one. If you want to charge your usage to a non-default GID (for example, s0901), add the GID to your PBS script. For example:

#PBS -W group_list=s0901

Understanding Queues

All NAS facility supercomputers use the Portable Batch System (PBS) to manage both interactive and batch jobs. Pleiades and Endeavour have separate PBS servers and job submission queues. Merope also has its own PBS server, but shares the **debug**, **normal**, and **long** queues with Pleiades.

Although different queues are available on different systems, queues typically have constraints on maximum wall-clock time and/or the number of nodes allowed for a job. Some queues have other constraints or are restricted to serving certain users or project ID numbers (GIDs). In addition, mission directorate limits are set on the number of cores available on Pleiades to ensure that each mission directorate can access a fair share of resources.

The following table lists commands you can use to view various types of queue information.

qstat -Q
List available queues and their constraints on a system
qstat -Qf
List available queues and their constraints on a system
qstat -W shares=-

List mission shares available for each mission

For more information, see the following articles:

- Queue Structure
- Preparing to Run on Endeavour
- Preparing to Run on Merope
- Pleiades Mission Shares Policy

HPC Environment Overview

Our HPC environment is operated by staff in the NASA Advanced Supercomputing (NAS) Division at Ames Research Center located at Moffett Field, CA. The supercomputers and support staff are funded by NASA's High-End Computing Capability (HECC) Project.

The topics in this section summarize the system components, such as the compute nodes, secure network connections, front-end systems, and data storage facilities; and the user environment, including information about the Linux operating system and the various filesystem directories that are available for your use.

Systems Overview

The systems available for your use are all protected within a secure environment. The figure below shows both the physical connections among all the components and their functional relationships through a typical user workflow. The environment is described in more detail in the following sections.

NUODiagram_KnowledgeBase_v9.jpg

The Secure Enclave

NAS supercomputing components are protected within a secure enclave that can be accessed only by authenticated users through the following secure bastions:

- Secure front ends (SFEs)
- Secure Unattended Proxy (SUP)
- DMZ file server

Components protected within the secure enclave include:

- Pleiades front-end (PFE) nodes
- Pleiades supercomputer
- Electra supercomputer
- Endeavour supercomputer
- Merope supercomputer
- Merope front-end system (mfe1)
- Lou mass storage system
- Lou front-end (LFE) nodes
- hyperwall visualization system
- Lou data analysis nodes (LDANs)

Note: Each user is provided with access and allocations for specific systems; some resources may not be available for your use.

The following sections give an overview of each component of the secure enclave.

Bastions

Secure Front Ends (SFEs)

The secure front ends (SFEs) provide inbound connection from your local system to the secure enclave. The first time you access the NAS systems within the enclave, you will authenticate through an SFE. Subsequently, you can use any of the bastions to access systems in the enclave.

For an overview of the initial authentication process, see <u>Logging in for the First Time</u>. For more information about the SFEs, see the article <u>Role of the Secure Front Ends</u>.

Secure Unattended Proxy (SUP)

The Secure Unattended Proxy (SUP) allows you to pre-authenticate to the secure enclave for one-week periods, during which you can perform unattended (batch) file transfers. After you complete the setup process, SUP is the most efficient and convenient method for transferring files from your remote system. For more information, see <u>Using the Secure Unattended Proxy (SUP)</u>.

DMZ File Server

A DMZ server is available for staging files between the NAS secure enclave and remote systems. The DMZ file server provides limited storage capacity to temporarily store files for very short durations. Files are automatically removed after 24 hours. For more information, see <u>File Staging through the DMZ File Server</u>.

Front Ends

The NAS supercomputers Pleiades, Electra, and Endeavour share the Pleiades front-end systems (PFEs). You can use the PFEs to edit files, compile your code, run short debugging and testing sessions, and submit batch jobs to the Pleiades and Electra compute nodes or to Endeavour. See the following articles for more information:

- Pleiades Front-End Usage Guidelines
- Pleiades Front-End Load Balancer

The Merope supercomputer uses its own front-end system, mfe1. You can use mfe1 to edit files, compile your code, run short debugging and testing sessions, and submit batch jobs to the Merope compute nodes. The Merope front-end system should not be used for pre- or post-processing tasks.

Compute Nodes

There are currently four supercomputers available for users: Pleiades, Electra, Endeavour, and Merope.

Pleiades

NASA's flagship supercomputer, and one of the most powerful production systems in the world, Pleiades is an SGI ICE cluster containing multiple generations of Intel processors. See the following articles for more information:

- General description of the <u>Pleiades supercomputer</u>
- Details on the <u>Pleiades configuration and usage guidelines</u>

Electra

Electra is NASA's first prototype modular supercomputing system, housed in an environmentally-friendly module located a short distance from the main NAS building. Electra uses the Pleiades front ends, filesystems, PBS server, and job gueues. See the following articles for more information:

- General description of the Electra supercomputer
- Details on the Electra configuration
- Preparing to Run on Electra

Endeavour

The Endeavour supercomputer is an SGI UV 2000 system that provides resources for user applications needing access to large cache-coherent, global shared-memory capabilities in a single system image (SSI). Endeavour uses the Pleiades front ends and filesystems, and shares some of the Pleiades InfiniBand fabric. However, Endeavour uses its own designated Portable Batch System (PBS) server and job queues. See the following articles for more information:

- General description of the Endeavour supercomputer
- Details on the Endeavour configuration
- Preparing to Run on Endeavour

Merope

Merope, a cluster comprised of repurposed Intel Xeon X5670 (Westmere) processors that were once part of Pleiades, is located in an auxiliary processing center about 3 kilometers from the NAS facility. Merope shares the home and scratch (/nobackup) filesystems with Pleiades, Electra, and Endeavour, but it uses its own designated front-end system and PBS server. See the following articles for more information:

- General description of the Merope supercomputer
- Details on the Merope configuration
- Preparing to Run on Merope

Note: The availability of Merope processor nodes varies, as they are also used for testing purposes.

Mass Storage System

The NAS facility provides long-term storage space on a single mass storage system, known as Lou. This SGI system has 2.9 petabytes (PB) of disk space and is capable of storing up to 132 PB on tape. The compute systems and the mass storage system combined have over 16 PB of disk storage on the floor. See the following articles for more information:

- Your Mass Storage Directory
- Lou Mass Storage System

Post-Processing Systems

Systems provided for post-processing include the Lou data analysis nodes (LDANs), designated as Idan[2-10] and the hyperwall visualization system. For a summary on using these systems for post-processing work, see Post-Processing Your Data. For detailed information, see also the following articles:

- Pleiades Front-End Usage Guidelines
- Lou Data Analysis Nodes
- Visualization System: hyperwall

Networks

The NAS high-speed network (NASLAN) includes a 10 gigabit-per-second (Gb/s) local area network and 10 Gb/s peering with other high-speed networks such as the NASA Integrated Communications Services (NICS), Internet2, and the Consortium for Educational Networks in California (CENIC). For an overview, see Networking Resources.

To access the HPC resources, you will use the <u>SSH protocol</u> to connect from your desktop system to a NAS bastion (usually the SFEs) through a wide area network and the NASLAN.

User Environment

All NAS systems run the Linux operating system. If you are new to Linux, you can find a lot of helpful information at the user-supported community website <u>Linux.org</u>, including a <u>Beginners Learning Course</u> that provides instruction on the basic directory structure of Linux, how to get around in the directories, how to access Linux documentation (man pages), useful commands, and much more. You can also find support at the Linux forum.

Note: SGI ProPack for Linux, which is designed to enhance the use of Linux on SGI systems, is installed on Pleiades and Endeavour. Merope runs the freely available Linux distribution CentOS, so an executable file built on Pleiades may need to be recompiled on Merope.

When your NAS account is created, your default Linux shell is set to be the C shell (csh); this is assumed to be the case throughout this guide. If you want to use a different shell as your default, such as bash, call the NAS Control Room staff at (800) 331-8737 or (650) 604-4444 or send an email message to support@nas.nasa.gov to request the change. After the change is made, the new default shell of your choice applies to all of your jobs.

Once you complete the initial setup for your NAS account, you will have access to the Pleiades and Merope front-end systems, the home filesystems, the Lou mass storage filesystems, and the scratch (/nobackup) filesystems. Your NAS account is authorized to run jobs on Pleiades, Endeavour, or both, depending on your allocation. Users with Pleiades allocations can run jobs on Pleiades, Electra, or Merope.

NAS supercomputers use the Portable Batch System (PBS) from Altair Engineering, Inc., for job submission, monitoring, and management. For more information about PBS, see <u>Submitting and Running Jobs</u>.

Filesystems

Pleiades, Electra, Endeavour, and Merope share the same home and scratch (/nobackup) filesystems. When you log into a PFE or the Merope front-end system, you will have access to the following directories:

- A home directory on the Pleiades home filesystem, which you can use to store a small number of files such as source code, small input files, and so on
- A /nobackup directory on a Lustre filesystem, which you can use to temporarily store larger files for reading and writing large amounts of data while running jobs

For long-term data storage, you also have access to a home directory on the Lou mass storage systems. The /nobackup filesystems are mounted on Lou, so you can easily copy files there directly from your /nobackup directory.

The Pleiades and Lou home filesystems are backed up each night. These backups are stored for approximately one year. The scratch (/nobackup) filesystems are *not* backed up.

Quota limits are enforced on all filesystems. Two kinds of quotas are supported:

- Limits on the total disk space occupied by your files
- Limits on the number of files you can store, irrespective of size; for quota purposes, directories count as files

See Quota Policy on Disk Space and Files for more information.

Your Home Directory

Your home directory is located on the Pleiades home filesystem, which is accessible from Pleiades, Electra, Endeavour, and Merope. Use your home directory to store a limited number of smaller files such as source code and input files. For temporary, short-term storage of larger files, use your /nobackup directory. For long-term data storage, use the Lou mass storage systems. See <u>Pleiades Home Filesystem</u> for more information.

Your Scratch (/nobackup) Directory

Use your /nobackup directory to temporarily store large files that read and write large amounts of data when you run jobs. Your /nobackup directory resides on one of several Lustre filesystems, designated /nobackuppX. To find out which Lustre filesystem your /nobackup directory is located on, run:

```
pfe20% ls -ld /nobackup/ your_nas_username
```

The /nobackup filesystems are also mounted on the Lou mass storage system, so you can access data in your /nobackup directory from Lou without going through Pleiades, Electra, Merope, or Endeavour.

WARNING: The /nobackup filesystems mean just that: they are not backed up. While this is stating the obvious, some users have lost important data by storing it on these systems over long periods of time. It is your responsibility to copy essential data to either your home directory, to archival storage on the Lou systems, or to your remote system.

See <u>Pleiades Lustre Filesystems</u> for more information.

Your Mass Storage Directory

For safe, long-term data storage, transfer your files to your Lou home directory. The Lou mass storage filesystem allows you to retrieve your stored files quickly and securely whenever you need them.

You can log into the Lou system just as you would any other NAS system and save data to mass storage by

copying your files to your Lou home directory: Lou:/u/your nas username.

NAS has no specified data-size quota for your Lou home directory, but you can store up to 250,000 files.

For more information, see <u>The Lou Mass Storage System</u>.

The Data Migration Facility

Data stored on Lou is migrated to tape, as needed, to make space on the disks for more data. Migrated files are retrieved to active disk when you attempt to read or write to them. These migration and retrieval processes are managed by SGI's Data Migration Facility (DMF), which also enables you to manually list, put, find, and get files that are on tape.

When your data is migrated to tape, two copies are written to two separate tape media in automated tape libraries located in two different buildings. See <u>Data Migration Facility Commands</u> for more information.

The Lou Filesystem

Lou is composed of the Lou front ends (LFEs), designated Ife[1-4]. The /nobackup filesystems are mounted on the LFEs, so you can easily copy files there directly from your /nobackup directory.

Although you cannot perform post-processing tasks on the LFEs, the Lou data analysis nodes provide PBS resources to perform post-processing tasks on your Lou mass storage data. For more information, see the following articles:

- The Lou Mass Storage System
- Lou Data Analysis Nodes

Software Modules

NAS provides software packages, such as compilers, pre- and post-processing programs, analysis tools, and math and scientific libraries. The software is managed through the use of modules that you can load into your home directories. To use modules, be sure to include the following line in your startup configuration file (for example, .cshrc), which contains information that is read by the Linux shell every time you log into the computer or open a new terminal window:

```
source /usr/local/lib/global.cshrc
```

Note: No default software is loaded on Pleiades, Endeavour, or Merope. If you want to automatically load a program when you log in, use the module load command in your startup configuration file.

For more information, see the following articles:

- Table of All Modules
- Customizing Your Environment